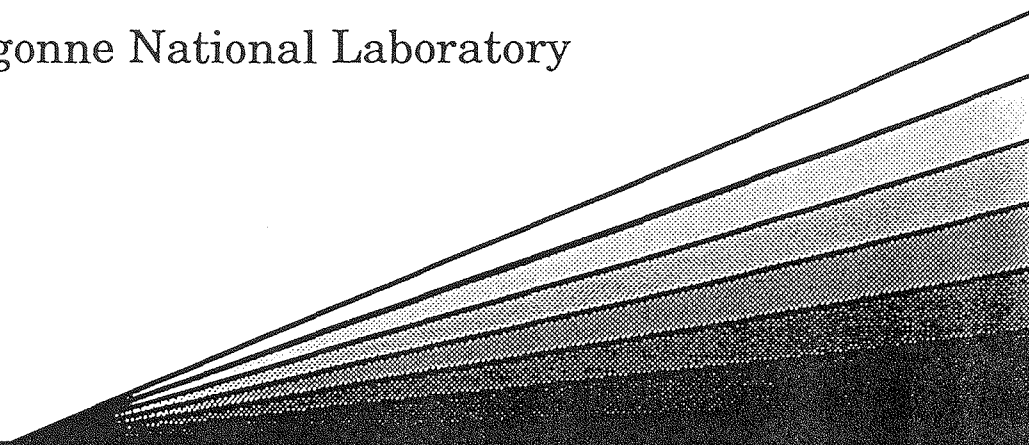# Emittance, Brilliance, and Bandpass Issues Related to an Inclined Crystal Monochromator

A. T. Macrander, D. R. Haeffner, and P. L. Cowan

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Argonne National Laboratory

EMITTANCE, BRILLIANCE, AND BANDPASS ISSUES RELATED TO AN INCLINED CRYSTAL MONOCHROMATOR[*]

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ABSTRACT

The inclined double crystal monochromator arrangement is very effective in handling high heat loads and holds considerable promise as a monochromator for undulator beams at third generation synchrotrons. Results for the ideal inclined crystal case have been obtained by dynamical diffraction calculations, and diffraction results for the (111) reflection of silicon are presented for an inclination angle of 85 ° and energies of 5 keV and 13.84 keV. The diffraction characteristics resemble closely diffraction from a symmetric (111) plane of silicon. However, the inclined and noninclined cases are not identical. Diffraction in the inclined case is slightly different due to refraction. The full width at half maximum of the Darwin-Prins reflectivity curve is slightly increased (~1%), and the angles of the outgoing beam after one reflection are slightly altered. That is, except for a wave incident at the Laue point in reciprocal space, the diffraction is always slightly asymmetric. The effect can be exactly reversed by an identical second crystal in the (+,-) arrangement.
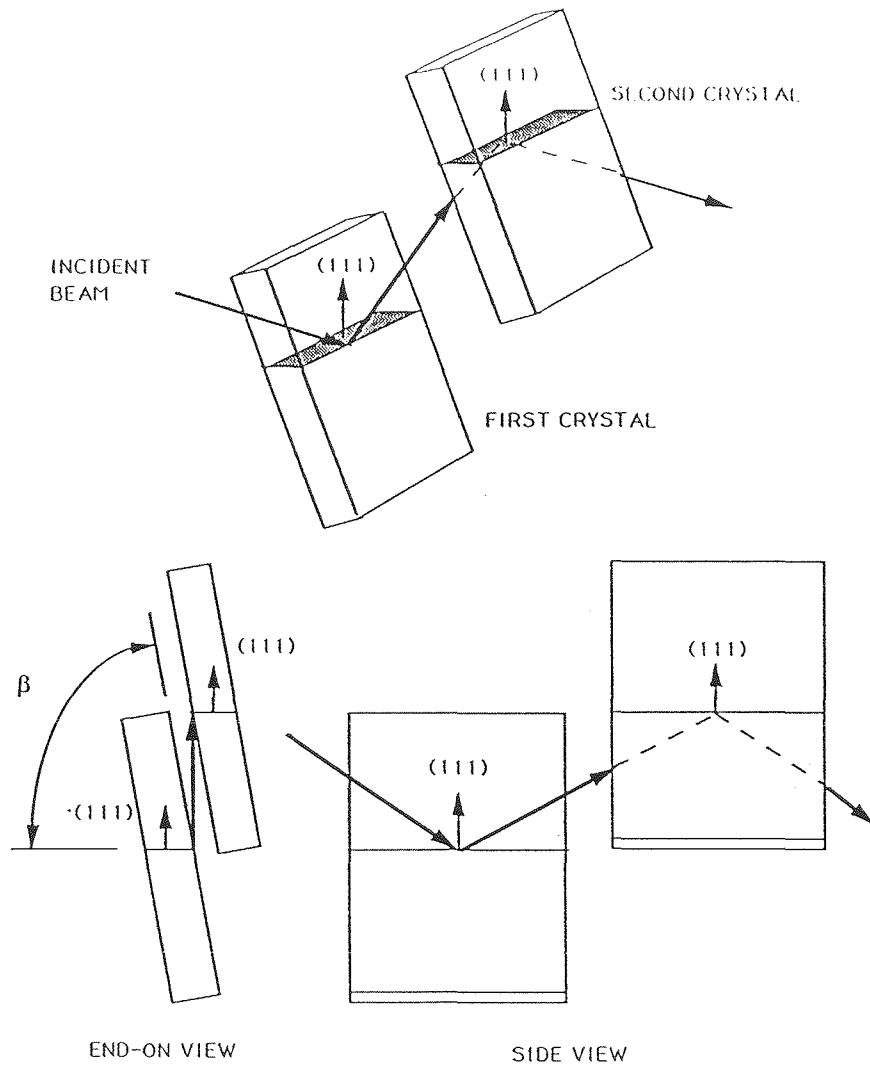
1. INTRODUCTION

Total power and power densities on crystal monochromators will reach unprecedented levels with the advent of undulator insertion devices at the Advanced Photon Source (APS). For example, present plans include a device with a 3.3 cm period that will deliver a total power of 3.8 kW with a peak power density of 148 W/mm^2. These heat loads imply severe thermal distortions in the crystal unless it is cooled.[1]

A recent optical innovation called an inclined crystal monochromator has also been tested under high heat load conditions.[2,3] In the inclined geometry (shown in Fig.1), the beam is incident at a small angle thereby spreading out the beam footprint. A significant reduction in the surface power density can be achieved without sacrificing the tuning range of the monochromator.

2. DISPERSION SURFACE TIE POINTS AND REFRACTION

The Bragg reflectivity of an ideal crystal can be calculated from x-ray dynamical diffraction theory. This is often done by assuming an incident plane wave and solving for tie points on the dispersion surface in reciprocal space.[4] A tie point is found by projecting the tail of the incident wave vector in a direction normal to the surface. In

INCIDENT
BEAM

SECOND CRYSTAL

(111)

(111)

FIRST CRYSTAL

β

(111)

·(111)

(111)

(111)

END-ON VIEW

SIDE VIEW

1. The inclined crystal geometry. The top portion of the figure shows a perspective view. The inclination angle is denoted as β.

the symmetric Bragg case for a coplanar set of incident wave vectors, this procedure yields tie points in a single diffraction plane. This is not the case, however, in the inclined geometry. At very high inclination angles, the projection normal to the inclined surface is almost parallel to the Bragg planes, and the tie points corresponding to the flanks of the Darwin curve are removed from the tie points for the symmetric Bragg case.

Differences in the direction of the exit beam are exacerbated the further one goes from the Laue point in reciprocal space. In particular, the beam corresponding to the center of the Darwin curve is affected because it is shifted away from the Laue point due to the average index of refraction. For this reason, we refer to the unusual effect of the inclined crystal boundary conditions on the direction of the exit beam as a refraction effect.
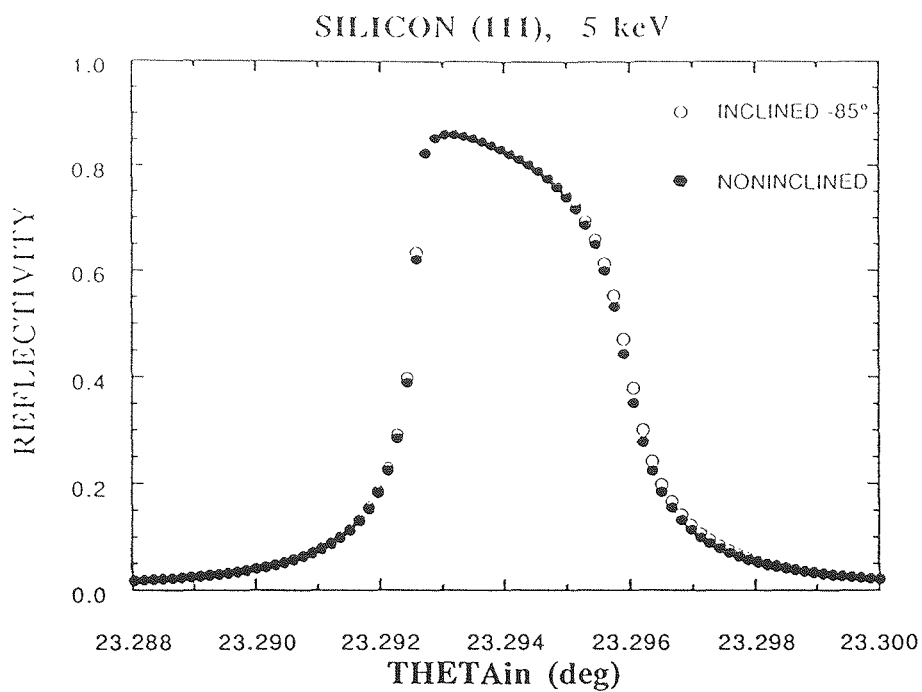
3. DARWIN-PRINS CURVES

We have applied dynamical diffraction theory to the inclined case. Two different calculations were made. In the first, a fourth-order expression for the dispersion surface was applied.[5] In the second, an 8x8 matrix technique that does not invoke reciprocal space[6] was applied. The matrix technique includes a reflected as well diffracted beams. Both methods yielded the result shown in Fig. 2 for the Darwin-Prins curve for 5 keV σ-polarized x-rays diffracted from the (111) planes of a silicon crystal inclined at 85 °. The curve for the standard symmetric Bragg Si(111) case is also shown, and the inclined case is seen to be very slightly broader (0.2 arcsec).

Due to plans at one of the beamlines at the APS to work at 13.84 keV, we have considered at length the optical properties of a Si(111), 85 ° inclined crystal monochromator at 13.84 keV. All the results at 13.84 keV were obtained using the 8x8 matrix technique and are for a σ polarized incident plane wave. The Darwin-Prins curve is shown in Fig. 3, and we note again that the inclined and standard symmetric diffraction cases give almost identical curves.

4. REFRACTION RESULTS

The unusual refraction effect is evident when one considers the direction of the outgoing beam. The angle that this beam makes with respect to the (111) Bragg planes (Θ_{out}) is slightly different from that of the incident beam (Θ_{in}). This is shown in Fig. 4. The effect is quite small; at the center of the reflectivity curve (i.e., at 8.2135°), the difference between Θ_{out} and Θ_{in} is only 0.14 arcsec. A bigger effect is found in the azimuthal rotation angle of the beam relative to the (111) direction. This angle is denoted as ρ and is shown in Fig. 5. For incident beams with ρ equal to zero the values of ρ for the corresponding exit beams are shown as a function of Θ_{in} in Fig. 6. The exit beams are all deflected away from the surface. The magnitude of the deflection at the center of the reflectivity curve is 0.03°. A slight lateral beamwalk given

SILICON (111), 5 keV

2. Darwin-Prins curves obtained from dynamical diffraction calculations at 5 keV. Noninclined corresponds to symmetric Bragg diffraction.

## SILICON (111), 13.84 keV
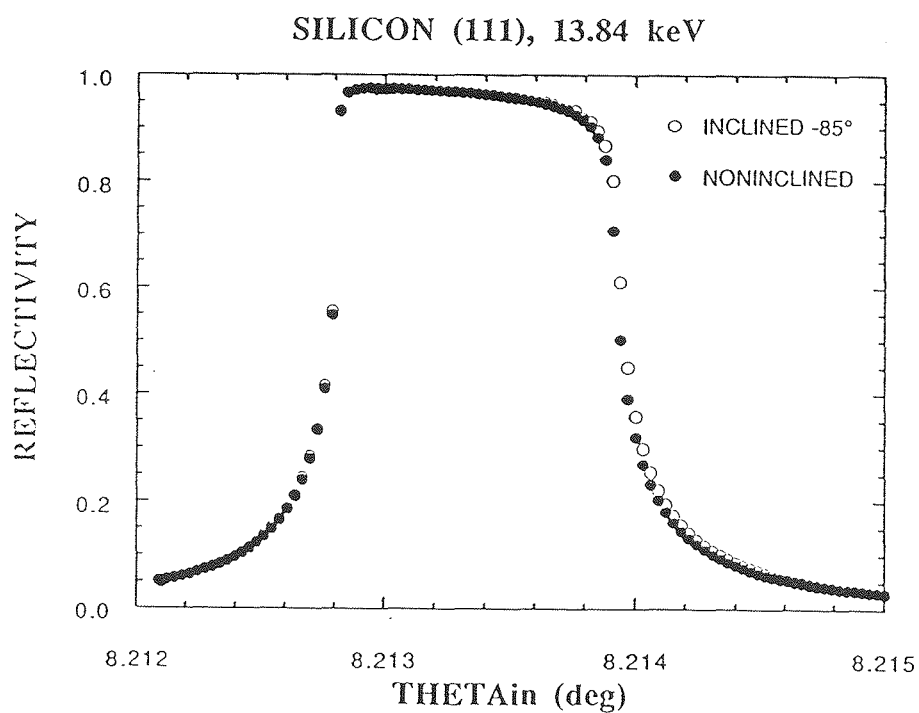
3. Darwin-Prins curves obtained from dynamical diffraction calculations at 13.84 keV.

SILICON (111), 85° INCLINED, 13.84 keV
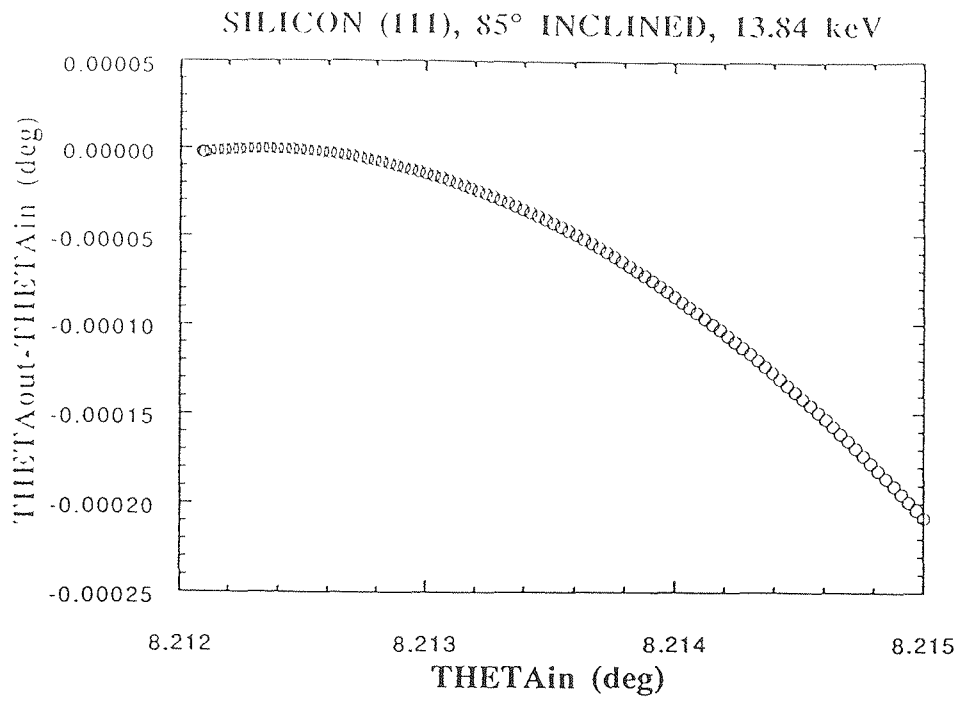
4. The difference between the angles of the ingoing and outgoing beams where the angles of the beams are measured with respect to the (111) plane.

SILICON (111), 85° INCLINED, 13.84 keV
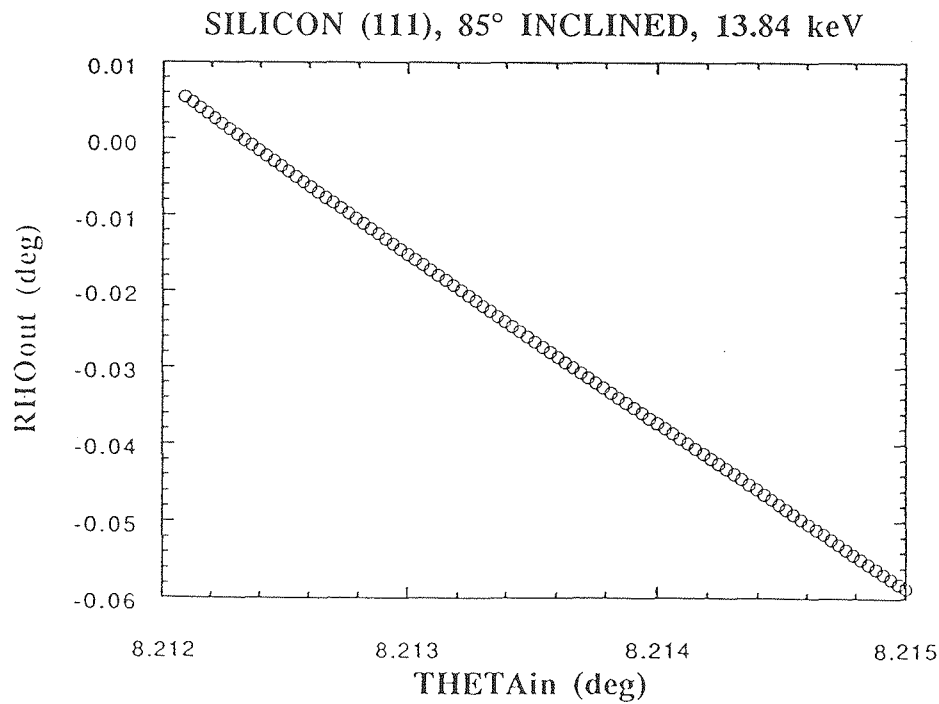
6. Values of ρ_{out} as a function of Θ_{in} for incident beams all having $\rho_{in}=0$.
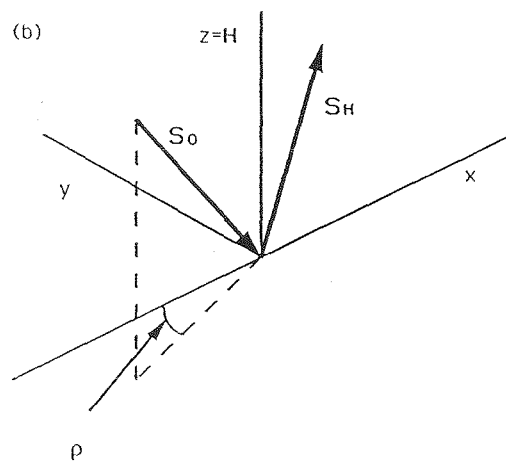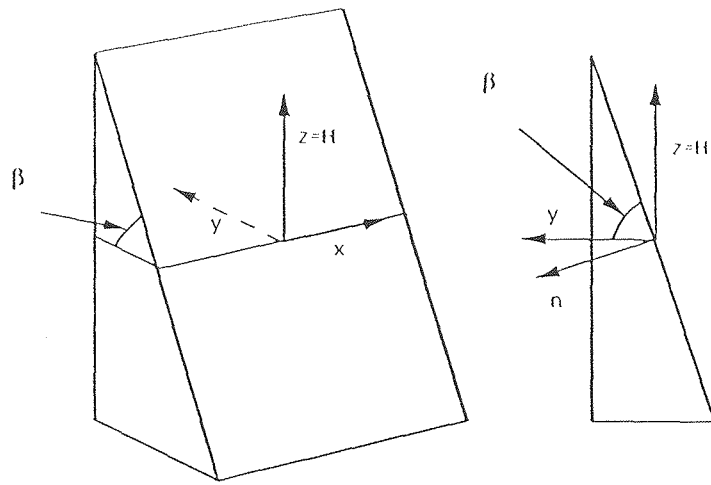
5. Definition of the azimuthal rotation angle around the reciprocal lattice vector (denoted as H) which is the [111] direction in the present calculations.

by Ltan (0.03°) is implied by these results, where L is the distance between the first and second crystals of a double crystal monochromator.

The effect of non-zero values of ρ_{in} on the width of the Darwin-Prins curve was considered previously under the assumption that $\Theta_{out} = \Theta_{in}$ and $\rho_{out} = \rho_{in}$.[7] The usual dynamical asymmetry factor known as b was calculated from geometrical arguments. The FWHM of the Darwin curve varies as $1/|b|^{0.5}$. In Fig. 7, compare the results obtained with this simple geometrical argument to results obtained with the 8x8 matrix technique. For values of ρ less than ~ -0.5°, total external reflection is approached, and, above ~ 0.7°, the exit beam is frustrated, i.e., it cannot escape from the crystal. The asymmetry in these two conditions arises from the deflection of the exit beam away from the surface. We see that, over most of the allowed range in ρ, the simple geometrical calculation gives practically the same value for the FWHM as does the rigorous dynamical matrix method. Only when total external reflection is approached are there significant differences. At the other end of the ρ range the two methods yield almost the same value for the width of the reflectivity curve, however, the reflectivity is significantly reduced. This is demonstrated in Fig. 8.

Finally, we have considered the bandpass of an inclined crystal reflection over the range of beam divergences anticipated for the central cone of APS Undulator A. The bandpass at zero divergence (i.e., ρ_{in} equals zero) was found to be 1.99 eV. This value is the same as for a standard symmetric reflection and does not change for divergences in the range 0 to 10 μrad, which covers the range of the central cone of the undulator.[8] The solution for the central cone shown in Fig. 9 is, consequently, not changed from that of a standard symmetric monochromator.
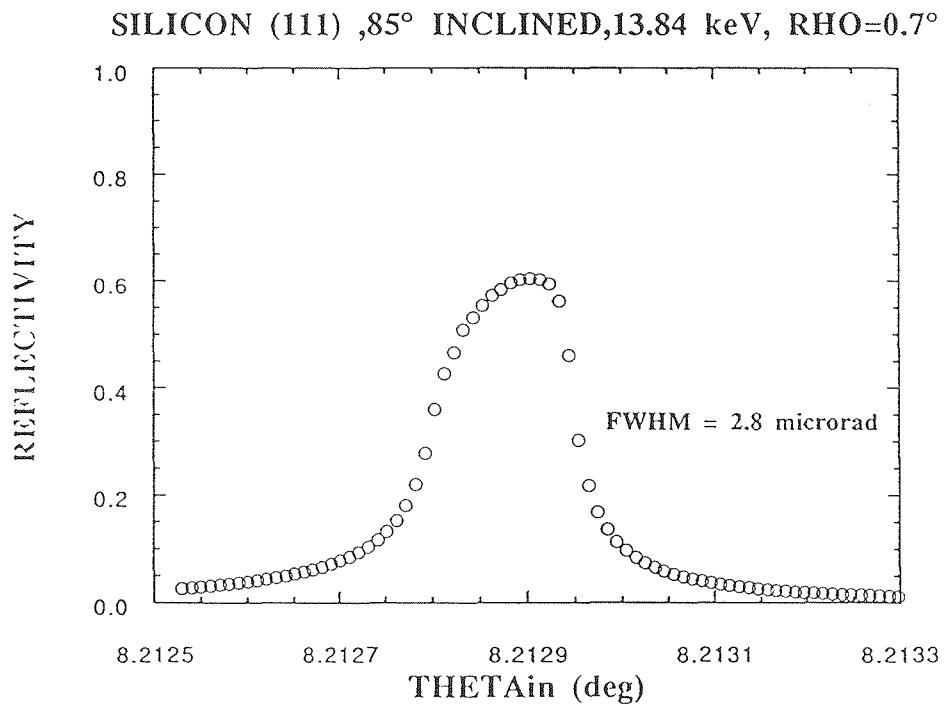
5. CONCLUSIONS

The net conclusion from all our dynamical calculations is that, unless one is operating at large azimuthal angles (ρ), the inclined crystal geometry does not significantly alter beam emittance, brilliance, or bandpass from that obtained with a standard symmetric double crystal monochromator. Furthermore, unless one is operating at incidence angles near the critical angle for total external reflection, the effect of the inclined crystal arrangement on the Darwin width can be closely approximated through the usual asymmetry factor (b). These angular limitations are far removed from the operating range anticipated for an inclined crystal monochromator at the APS.

6. ACKNOWLEDGMENTS

SILICON (111), 85° INCLINED, 13.84 keV
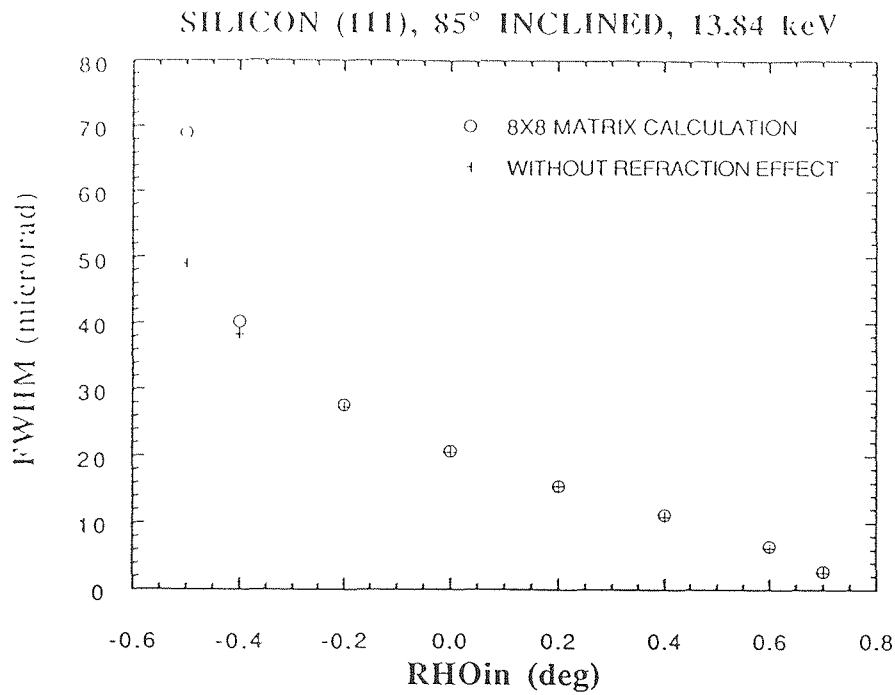
7. FWHM values of Darwin-Prins curves as function of ρ_{in}. Values which ignore the refraction effect were obtained by using simple geometric arguments and by assuming that Θ_{out} equals Θ_{in} and that ρ_{out} equals ρ_{in} (see. Ref. 7).

SILICON (111) ,85° INCLINED,13.84 keV, RHO=0.7°

FWHM = 2.8 microrad

8. Darwin-Prins curve under conditions for which the exit beam is partially frustrated.
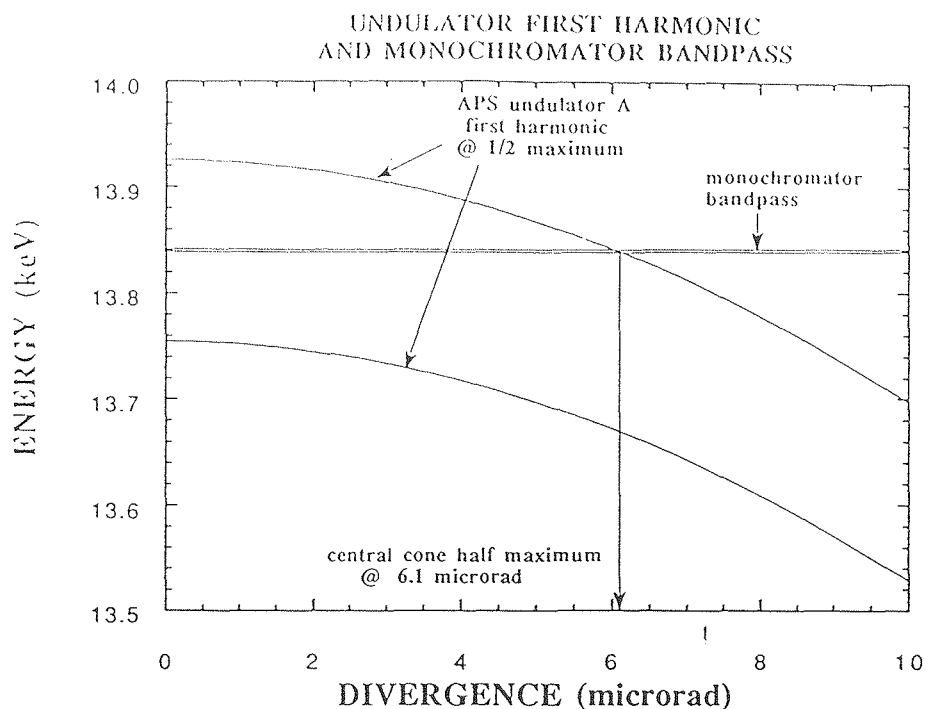
9. Graphical solution of the central cone half maximum for APS undulator A with a Si(111) monochromator.

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